

Cu<sub>6</sub>Bi[AsO<sub>4</sub>]<sub>3</sub>[OH]<sub>6</sub>[H<sub>2</sub>O]

hP86

(176)  $P6_3/m - i^4h^6d$ **BiCu<sub>6</sub>(AsO<sub>4</sub>)<sub>3</sub>(OH)<sub>6</sub>·H<sub>2</sub>O** [1], mixite partly dehydrated

Structural features: BiO<sub>6</sub>(OH)<sub>3</sub> tricapped trigonal prisms share vertices with AsO<sub>4</sub> tetrahedra to form infinite columns, which are interconnected via ribbons of edge-linked Cu(O<sub>2</sub>[OH]<sub>2</sub>) squares to form a 3D-framework; H<sub>2</sub>O in channels parallel to [001] (partial disorder).

Miletich R. et al. (1997) [1]

As<sub>3</sub>BiCu<sub>6</sub>H<sub>8</sub>O<sub>19</sub> $a = 1.3631$ ,  $c = 0.5905$  nm,  $c/a = 0.433$ ,  $V = 0.9502$  nm<sup>3</sup>,  $Z = 2$ 

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
(OH <sub>2</sub> )1	12 <i>i</i>	1	0.073	0.191	0.109	0.042	single atom (OH <sub>2</sub> )
O2	12 <i>i</i>	1	0.1776	0.5727	0.0175		single atom As
(OH <sub>2</sub> )3	12 <i>i</i>	1	0.195	0.027	0.083	0.083	single atom (OH <sub>2</sub> )
Cu4	12 <i>i</i>	1	0.31399	0.41039	0.00254		square pyramid (OH) <sub>2</sub> O <sub>3</sub>
O5	6 <i>h</i>	<i>m</i> ..	0.0075	0.3993	<sup>1</sup> / <sub>4</sub>		non-coplanar triangle AsCu <sub>2</sub>
As6	6 <i>h</i>	<i>m</i> ..	0.14978	0.49348	<sup>1</sup> / <sub>4</sub>		tetrahedron O <sub>4</sub>
(OH <sub>2</sub> )7	6 <i>h</i>	<i>m</i> ..	0.185	0.164	<sup>1</sup> / <sub>4</sub>	0.083	non-colinear (OH <sub>2</sub> ) <sub>2</sub>
O8	6 <i>h</i>	<i>m</i> ..	0.2158	0.4146	<sup>1</sup> / <sub>4</sub>		non-coplanar triangle AsCu <sub>2</sub>
(OH)9	6 <i>h</i>	<i>m</i> ..	0.3752	0.3695	<sup>1</sup> / <sub>4</sub>		non-colinear Cu <sub>2</sub>
(OH)10	6 <i>h</i>	<i>m</i> ..	0.4403	0.1961	<sup>1</sup> / <sub>4</sub>		non-colinear Cu <sub>2</sub>
Bi11	2 <i>d</i>	-6..	<sup>2</sup> / <sub>3</sub>	<sup>1</sup> / <sub>3</sub>	<sup>1</sup> / <sub>4</sub>		tricapped trigonal prism O <sub>6</sub> (OH) <sub>3</sub>

Transformation from published data: origin shift 0 0 <sup>1</sup>/<sub>2</sub>

Experimental: single crystal, diffractometer, X-rays, R = 0.036

Remarks: Synthetic mixite, partly dehydrated under flowing nitrogen. Short interatomic distances for partly occupied site(s). Hydrogen atoms are not taken into consideration for Pearson symbol, Wyckoff sequence and atomic environments.

References: [1] Miletich R., Zemmann J., Nowak M. (1997), Phys. Chem. Miner. 24, 411-422.